Topological effects in QCD and the problem of short-distance singularities

Martin Lüscher

CERN, Physics Department, TH Division
CH-1211 Geneva 23, Switzerland

Abstract

The topological susceptibility and the higher moments of the topological charge distribution in QCD are expressed through certain n-point functions of the scalar and pseudo-scalar quark densities at vanishing momenta, which are free of short-distance singularities. Since the normalization of the correlation functions is determined by the non-singlet chiral Ward identities, these formulae provide an unambiguous regularization-independent definition of the moments and thus of the charge distribution.

1. Quantum fields are subject to random fluctuations and are therefore not an obvious case for the application of topological arguments. In the presence of a smooth background field, and if the quantum fluctuations are treated perturbatively, the problem usually remains unnoticed, because the topological information is entirely encoded in the background field. In general a separation of the fluctuations is not possible, however, and in these situations it may be difficult to give an unambiguous meaning to the notion of, say, a topological sector.

In QCD the axial anomaly provides a link between the correlation functions of local fields and the topology of the underlying classical field space. Large-N counting rules and the anomalous chiral Ward identities lead to the Witten–Veneziano formula [1–4], for example, which relates the vacuum expectation value of the square of the topological charge

$$Q = \int \mathrm{d}^4x \, q(x), \qquad q(x) \equiv -\frac{1}{32\pi^2} \, \epsilon_{\mu\nu\rho\sigma} \mathrm{tr}\{F_{\mu\nu}(x)F_{\rho\sigma}(x)\}, \tag{1.1}$$

(where $F_{\mu\nu}$ denotes the field strength of the gauge field) to the mass of the η' meson. More recently, when studying QCD in the so-called ϵ-regime [5], the Ward identity was used to trade the topological term in the partition function

$$\mathcal{Z}(\theta) = \int_{\text{fields}} \mathrm{e}^{-S+i\theta Q} \tag{1.2}$$

for a phase factor in the quark mass term in the action S. Close to the chiral limit, and at any value of θ, the theory may then be described by the standard effective chiral σ-model [6]. An interesting point to note here is that, in the effective theory, it is possible to define fixed-charge correlation functions by keeping only the terms proportional to a given power of $\mathrm{e}^{i\theta}$ in the chiral expansions of the partition function and the unnormalized correlation functions.

For the reasons indicated above, the situation in QCD is more complicated in this respect. Technically the difficulty is that the topological susceptibility

$$\chi_t = \int \mathrm{d}^4x \, \langle q(x)q(0) \rangle \tag{1.3}$$

and the higher derivatives of the free energy $F(\theta) = -\ln \mathcal{Z}(\theta)$ involve an integration of correlation functions with non-integrable short-distance singularities. In eq. (1.3), for example, the integrand diverges like $(x^2)^{-4}$ (up to logarithms). If no subtraction prescription is specified, the free energy is therefore ill-defined, and so are the fixed-charge correlation functions of local fields.

It is sometimes pointed out in this connection that the charge density is equal to the divergence of the Chern–Simons current and that this would allow the integral to be rewritten in the form of a surface integral. While the short-distance singularities are avoided in this way, the argument requires the gauge to be fixed and is hence difficult to put on solid grounds beyond perturbation theory.

2. In lattice QCD various definitions of the topological susceptibility were proposed over the years, but it remained unclear which of these (if any) would have the correct continuum limit. The question is in fact undecidable as long as there is no unambiguous definition of the susceptibility in the continuum theory.

The charge density may be represented on the lattice by any local composite field of dimension 4 with the appropriate symmetry properties. In general the topological character of the charge density is lost, however, and the topological susceptibility consequently does not vanish in perturbation theory (and therefore diverges proportionally to the fourth inverse power of the lattice spacing) [7]. To avoid this singular behaviour one would like the charge density on the lattice to be such that the associated charge is invariant under smooth deformations of the gauge field. In the classical continuum theory, the density is, incidentally, completely determined by this condition up to divergence terms $\partial_\mu k_\mu$ (where k_μ is any gauge-invariant local current) and a normalization factor [8,9].

Lattice representations of the charge density that preserve its topological character were constructed a long time ago [10,11]. Unfortunately these constructions are not unique, because the space of lattice gauge fields is connected and its division into charge sectors is therefore arbitrary to some extent. Since there is an action barrier between the sectors, it seems likely, however, that the regions in field space around the sector boundaries become irrelevant close to the continuum limit. Whether the topological susceptibility is finite in this limit is then a second issue that remains to be discussed.

If one of the formulations of lattice QCD that preserve chiral symmetry is used, there is a natural definition of the charge density that is topological in the sense explained above and that appears in the flavour-singlet chiral Ward identities, exactly as in the continuum theory [12–21]. For this case, and if there are 3 or more mass-degenerate quark flavours, Giusti, Rossi and Testa [22] recently showed that the topological susceptibility is at most logarithmically divergent in the continuum limit, i.e. that all power-divergent contributions cancel.

In the present paper the argumentation of ref. [22] is cast in a slightly different and more general form. This leads to an alternative representation of the susceptibility and the higher-order moments of the charge distribution, which remains well-defined

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in the continuum limit. The lattice regularization is then no longer needed and the final formulae (which are free of short-distance singularities) may be taken as the field-theoretic definition of the susceptibility and the higher moments.

3. In the following we consider QCD with any number N_f of massive quarks. Space-time is assumed to be a finite periodic box, but in many equations it will be straightforward to pass to the infinite-volume limit since the theory has a mass gap. We now first derive a new representation of the topological susceptibility on the lattice and shall return to the continuum theory in the next section.

The lattice theory is set up on a hypercubic lattice with spacing a, using a (massless) lattice Dirac operator D that satisfies the Ginsparg–Wilson relation

$$\gamma_5 D + D\gamma_5 = aD\gamma_5 D \qquad (3.1)$$

and the usual symmetry, hermiticity and regularity requirements †. As explained in ref. [21], the suggested choice of the quark action in this formulation of lattice QCD reads

$$S_F = a^4 \sum_{x,r} \overline{\psi}_r(x) D_{m_r} \psi_r(x), \qquad D_m \equiv (1 - \tfrac{1}{2}am)D + m, \qquad (3.2)$$

where the index r labels the quark flavours and $m_1, \ldots, m_{N_f}$ are the associated bare quark masses. Most other details of the lattice theory (the action of the gauge field for example) are left unspecified since we will not need to know them.

The scalar and pseudo-scalar quark densities that transform like a $U(N_f) \times U(N_f)$ multiplet under the exact chiral symmetries of the lattice action (3.2) are given by

$$S_{rs}(x) = \overline{\psi}_r(x)(1 - \tfrac{1}{2}aD)\psi_s(x), \qquad (3.3)$$

$$P_{rs}(x) = \overline{\psi}_r(x)\gamma_5(1 - \tfrac{1}{2}aD)\psi_s(x). \qquad (3.4)$$

Keeping track of the flavour indices in this way rather than introducing a basis of group generators will simplify the discussion in the following.

As is the case in the continuum theory, the flavour-singlet chiral transformations are anomalous on the lattice, the anomaly being proportional to the topological

† The Dirac matrices γ_μ are taken to be hermitian and $\gamma_5 = -\gamma_0\gamma_1\gamma_2\gamma_3$. Whenever possible the same symbols are used for the fields (and other items) in the continuum theory and on the lattice since it is usually clear from the context which one is meant.

charge density

$$q(x) = -\tfrac{1}{2}a\,\mathrm{tr}\{\gamma_5 D(x,x)\}. \tag{3.5}$$

In this equation, $D(x,y)$ stands for the kernel of the lattice Dirac operator in position space and the little trace "tr" is taken over the Dirac and colour indices only. The normalizations are such that the associated charge

$$Q = a^4 \sum_x q(x) \tag{3.6}$$

is equal to the index of the Dirac operator [17].

A well-known consequence of the Ginsparg–Wilson relation and the γ_5-hermiticity of the Dirac operator is that, for any given gauge field, there exists an orthonormal basis of eigenfunctions of D with eigenvalues λ of the form

$$\lambda = \frac{1}{a}\left(1 - e^{i\alpha}\right), \quad \alpha \in \mathbb{R}. \tag{3.7}$$

Now if $f(\lambda)$ is any bounded function on the spectral circle (3.7), the identity

$$\mathrm{Tr}\{\gamma_5 f(D)\} = \{f(0) - f(2/a)\}\,Q \tag{3.8}$$

is easily established by evaluating the trace in the basis of eigenfunctions χ of D, noting that $\gamma_5\chi$ is orthogonal to χ if the associated eigenvalue λ is not real.

Using this general result, a variety of formulae for the topological charge can be obtained. We may, for example, start from the equation

$$a^{4r} \sum_{x_1,\dots,x_r} \langle P_{r1}(x_1)S_{12}(x_2)\dots S_{r-1\,r}(x_r)\rangle_{\mathrm{F}} =$$

$$-\mathrm{Tr}\{\gamma_5(1 - \tfrac{1}{2}aD)(D_{m_1})^{-1}\dots(1 - \tfrac{1}{2}aD)(D_{m_r})^{-1}\} \tag{3.9}$$

in which $\langle\dots\rangle_{\mathrm{F}}$ denotes the fermion expectation value (the Wick contraction) of the fields in the bracket. The application of the trace identity (3.8) then yields

$$Q = -m_1\dots m_r \times a^{4r} \sum_{x_1,\dots,x_r} \langle P_{r1}(x_1)S_{12}(x_2)\dots S_{r-1\,r}(x_r)\rangle_{\mathrm{F}} \tag{3.10}$$

for all $r \leq N_{\mathrm{f}}$.

It is now immediate that

$$\chi_t = m_1 \ldots m_s \times a^{4s-4} \sum_{x_1,\ldots,x_{s-1}} \big\langle P_{r1}(x_1)S_{12}(x_2)\ldots S_{r-1\,r}(x_r)$$

$$\times P_{s\,r+1}(x_{r+1})S_{r+1\,r+2}(x_{r+2})\ldots S_{s-1\,s}(0)\big\rangle_{\mathrm{c}} \tag{3.11}$$

if r, s are in the range $1 \le r < s \le N_{\mathrm{f}}$. In this formula, $\langle\ldots\rangle_{\mathrm{c}}$ denotes the full QCD connected correlation function of the local fields in the bracket and the flavour labels are such that the contraction of the quark fields results in a product of two fermion loops (one for each factor of the topological charge).

4. Assuming for a moment that there are at least 5 quark flavours, we are thus led to tentatively write

$$\chi_t = m_1 \ldots m_5 \int \mathrm{d}^4x_1 \ldots \mathrm{d}^4x_4 \big\langle P_{31}(x_1)S_{12}(x_2)S_{23}(x_3)P_{54}(x_4)S_{45}(0)\big\rangle_{\mathrm{c}} \tag{4.1}$$

for the topological susceptibility in the continuum theory. Power counting and the operator product expansion now suggest that the correlation function in this expression does not have any non-integrable short-distance singularities. The dimensionality of the correlation function certainly excludes such a singularity if all coordinates are scaled to a common point. If only some coordinates are scaled, the corresponding field product converges to a local field of dimension 3 or more, and the dimensional analysis then again shows that there is no non-integrable singularity.

A second observation is that the normalization of the products $m_r P_{st}$ and $m_r S_{st}$ is determined by the non-singlet chiral Ward identities. Equation (4.1) thus provides an unambiguous regularization-independent definition of the topological susceptibility in the continuum theory (if there are 5 or more flavours of quarks). Moreover we may conclude that the susceptibility on the lattice, as defined in section 3, is finite in the continuum limit and that its value in the limit is given by eq. (4.1).

It may be reassuring to note at this point that trace identities similar to those we have used on the lattice hold in the continuum theory too. In the presence of a smooth background gauge field, the massless Dirac operator D has all its eigenvalues λ on the imaginary axis in this case, and if $f(\lambda)$ is any continuous function that decays rapidly enough at infinity, it can be shown that

$$\mathrm{Tr}\{\gamma_5 f(D)\} = f(0)Q. \tag{4.2}$$

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A relatively easy proof of the Atiyah–Singer index theorem actually starts from the observation that

$$\mathrm{Tr}\big\{\gamma_5 \mathrm{e}^{tD^2}\big\} = \mathrm{index}(D) \tag{4.3}$$

for any $t > 0$. In the limit $t \to 0$, the trace can then be worked out, using heat kernel techniques, and is found to be equal to the topological charge of the background field [23]. The application of eq. (4.1) in a semi-classical context is therefore guaranteed to give results consistent with naive expectations.

5. The higher connected moments

$$C_n = a^{8n-4} \sum_{x_1,\dots,x_{2n-1}} \big\langle q(x_1)\dots q(x_{2n-1})q(0)\big\rangle_{\mathrm{c}} \tag{5.1}$$

of the charge distribution on the lattice can also be rewritten in a form that remains well-defined in the continuum limit. Assuming again that there are at least 5 quark flavours, we have

$$C_n = m_1\dots m_5 \times a^{8n+8} \sum_{x_1,\dots,x_{2n+2}} \big\langle P_{31}(x_1)S_{12}(x_2)S_{23}(x_3)P_{54}(x_4)S_{45}(x_5)$$

$$\times q(x_6)\dots q(x_{2n+2})q(0)\big\rangle_{\mathrm{c}}. \tag{5.2}$$

This formula is not quite what we need (some sub-leading non-integrable singularities are still present), but we may now eliminate the remaining factors of the topological density by applying the exact chiral Ward identity [19]

$$a^4 \sum_x \big\langle \{q(x) + m_1 P_{11}(x)\}\,\mathcal{O}\big\rangle_{\mathrm{c}} = \tfrac{1}{2}\big\langle \delta\mathcal{O}\big\rangle_{\mathrm{c}} \tag{5.3}$$

a number of times, where $\delta\mathcal{O}$ derives from the transformation law

$$\delta\psi_1 = \gamma_5(1 - aD)\psi_1, \qquad \delta\overline{\psi}_1 = \overline{\psi}_1\gamma_5. \tag{5.4}$$

As a result, a sum of connected expectation values of products of $m_r P_{st}$ and $m_r S_{st}$ with 5 or more factors is obtained, all of which have only integrable short-distance singularities in the continuum theory (it should be noted here that the constant field does not contribute to the operator product expansion in a connected correlation function if only some coordinates are scaled to a common point). The bottom line

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is then that the moments C_n are finite in the continuum limit (if $N_{\mathrm{f}} \geq 5$) and that their values in the limit can, in principle, be determined without recourse to any particular regularization of the theory.

6. For real-world QCD the condition that there should be at least 5 flavours of quarks is not a limitation, but it seems a bit strange that the bottom quark must be involved in order to define the topological susceptibility in the continuum theory. The constraint on the number of quark flavours can in fact be relaxed by introducing a multiplet of valence quarks.

In the extreme case of the pure gauge theory, for example, the fermion action on the lattice is then given by

$$S_{\mathrm{F}} = a^4 \sum_x \left\{ \sum_{r=1}^{2N} \overline{\psi}_r(x) D_m \psi_r(x) + \sum_{k=1}^{N} |D_m \phi_k(x)|^2 \right\}, \tag{6.1}$$

where $\overline{\psi}_r, \psi_r$ are the valence quark fields and ϕ_k the associated pseudo-fermion fields. For positive quark masses m, a well-defined euclidean field theory is obtained in this way that is probably not reflection-positive, but in which power-counting arguments and the operator product expansion can be expected to apply, since the locality of the theory is preserved.

We may now again make use of the trace identities to rewrite the moments C_n of the charge distribution in terms of correlation functions of the scalar and pseudo-scalar quark densities. The discussion of the short-distance singularities is, however, slightly modified with respect to the case of full QCD, because the pseudo-fermion fields allow for the construction of flavour-singlet fields of dimension 2. On the other hand, we can take advantage of the fact that there is no constraint on the number of valence quarks (the charge distribution is always the same), and it is then easy to show that the expression

$$C_n = m^{6n} a^{24n-4} \sum_{x_1,\ldots,x_{6n-1}} \big\langle P_{31}(x_1) S_{12}(x_2) S_{23}(x_3) P_{64}(x_4) S_{45}(x_5) S_{56}(x_6) \ldots$$

$$\ldots P_{6n\,6n-2}(x_{6n-2}) S_{6n-2\,6n-1}(x_{6n-1}) S_{6n-1\,6n}(0) \big\rangle_{\mathrm{c}} \tag{6.2}$$

is finite in the continuum limit.

It may be worth mentioning here that we never had to refer to the chiral limit in this section and that one is free to set the renormalized valence quark mass to any fixed physical value. This saved us from some difficult questions, since the true asymptotic chiral behaviour of valence quarks is still not known.

Equation (6.2) can also be written in the more suggestive form

$$C_n = V^{-1}\big\langle (Q_{\mathrm{F}})^{2n} \big\rangle_{\mathrm{c}}, \tag{6.3}$$

$$Q_{\mathrm{F}} \equiv -m^3 a^6 \sum_{x_1,x_2,x_3} \langle P_{31}(x_1)S_{12}(x_2)S_{23}(x_3)\rangle_{\mathrm{F}}, \tag{6.4}$$

where V denotes the space-time volume. In terms of the valence quark propagator, Q_{F} is simply equal to the triangle graph with one pseudo-scalar and two scalar vertices and vanishing external momenta. The important point is that these equations apply independently of the chosen regularization, provided the fields and the quark mass are renormalized in accordance with the non-singlet chiral Ward identities.

7. Beyond the semi-classical regime, the universality of the moments of the topological charge distribution (and thus of the distribution itself) derives from a combination of fundamental properties of QCD. Asymptotic freedom was implicitly used, for example, when applying the operator product expansion to show the absence of non-integrable short-distance singularities in the final formulae for the moments. In the way the problem was approached here, a key rôle was also played by the trace identities (3.8) on the lattice and (4.2) in the continuum theory. To some extent at least, these identities can be understood as an algebraic reflection of the fact that the index of the Dirac operator is a homotopy invariant.

If a lattice formulation of QCD that preserves chiral symmetry is used, the naive definition of the topological susceptibility and the higher moments coincides with the universal definition in the continuum limit through the finite expressions that were obtained in this paper. This result is quite important, from both the conceptual and the practical points of view, and it also closes a gap in the recent literature on the topological susceptibility and the ϵ-regime (see ref. [24], for example, and references quoted there). Evidently there is no reason to expect the same to be true if other formulations of lattice QCD and other definitions of the topological charge density are considered. The moments can, however, always be defined through the universal formulae, and some of these may actually be quite accessible to numerical simulations.

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